





a cytokine, a lymphokine, a chemokine, an adhesion molecule, a growth factor, and a receptor thereof.

10. (Withdrawn) The method of claim 9, wherein the target protein is a receptor.

11. (Withdrawn) The method of claim 9, wherein the receptor is a member of the TNF receptor superfamily.

12. (Withdrawn) The method of claim 11, wherein the TNF receptor superfamily member is selected from the group consisting of the TNF receptor, fas, CD40, gp120, fas ligand, TNF- $\alpha$ ,  $\beta$ -lactamase, c-erbB2, growth hormone receptor, growth hormone, insulin receptor, insulin, IL-1 receptor, IL-1, IL-2 receptor, IL-2, epidermal growth factor receptor (EGFR), and epidermal growth factor.

13. (Withdrawn) The method of claim 12, wherein the TNF receptor superfamily member is a TNF receptor.

14. (Withdrawn) The method of claim 9, wherein the target protein is an enzyme.

15. (Withdrawn) The method of claim 14, wherein the enzyme is  $\beta$ -lactamase.

16. (Withdrawn) The method of claim 9, wherein the target protein is a member of the immunoglobulin superfamily.

17. (Withdrawn) The method of claim 16, wherein the target protein is CD4.

18. (Withdrawn) The method of claim 1 wherein the modifier is a protein, a non-proteinaceous molecule, or a non-organic molecule.





d) testing said compounds in an in vitro assay to detect a compound which modulates the interaction at the functionally critical site between said target protein and said modifier.

28. (New) A method of identifying a compound that is an allosteric modulator of an intermolecular interaction associated with a predetermined biological function to be modulated, said interaction occurring between a target protein and a modifier at a functionally critical site on a target protein, which method comprises:

a) identifying an allosteric cavity that is a measurable distance on the target protein from the functionally critical, said cavity being a candidate site for accommodating an allosteric modulator;

b) calculating the dimensions of said cavity;

c) mapping the chemical and/or electrostatic properties of said cavity;

d) identifying compounds that contain functional groups that can be accommodated by said cavity;

e) testing said compounds in an in vitro assay to detect a compound which modulates the interaction at the functionally critical site between said target protein and said modifier;

thereby identifying a compound that is an allosteric modulator of the interaction at the functionally critical site between said target protein and a modifier.

29. (New) A method of identifying a compound that is an allosteric modulator of an intermolecular interaction at a functionally critical site on a target protein, wherein the intermolecular interaction at the functionally critical site is between the target protein and a modifier, and wherein the interaction is associated with a predetermined biological to be modulated, which method comprises:

a) identifying an allosteric cavity on a target protein that is a measurable distance from the functionally critical site on the target protein, said cavity being a candidate site for accommodating an allosteric modulator;

b) calculating the dimensions of said cavity and mapping the chemical and/or electrostatic properties of said cavity;

c) identifying compounds that contain functional groups that can be accommodated by said cavity;

d) testing said compounds in an in vitro assay to detect a compound which modulates the interaction at the functionally critical site between said target protein and said modifier;

thereby identifying a compound that is an allosteric modulator of the interaction at the functionally critical site between said target protein and a modifier.

30. (New) A method of identifying a compound that is an allosteric modulator of an intermolecular interaction at a functionally critical site, wherein the functionally critical site is the site of the intermolecular interaction between a target protein and a modifier that is necessary for the specific biological function attributed to the target protein, which method comprises the steps of

a) identifying an allosteric cavity on a target protein that is a measurable distance from the functionally critical site on the target protein, said cavity being a candidate site for binding an allosteric modulator;

b) calculating the dimensions of said cavity and mapping the chemical and/or electrostatic properties of said cavity;

c) identifying compounds that contain functional groups that can be accommodated by said cavity;

d) testing said compounds in an in vitro assay to detect a compound which modulates the interaction at the functionally critical site between said target protein and said modifier;

thereby identifying a compound that is an allosteric modulator of the interaction at the functionally critical site between said target protein and a modifier.